Westfälische Wilhelms-Universität Münster

Center for Nonlinear Science

Münsteranian Torturials on Nonlinear Science

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Continuation

HETDRIV : Steady drops on a heterogeneous substrate under lateral driving

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with the support of

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www.uni-muenster.de/CeNoS/Lehre/Tutorials/auto.html

1 hetdriv: Steady drops on a heterogeneous substrate under lateral driving

The tutorial HETDRIV explores steady drops on a surface with heterogeneous wettability under the influence of lateral driving. You will calculate these steady states as a function of continuation parameters: domain length, heterogeneity strength and driving parameter.

1.1 Model

This tutorial illustrates the calculation of pinned steady drop solutions of the dimensionless thin film equation

$$\partial_t h \;=\; -\partial_x \left\{ Q(h)\,\partial_x \left[\underbrace{\partial_{xx}h - \partial_h f(h,x)}_{\text{pressure term}} \right] + \chi(h) \right\} 6 \tag{1.1}$$

For an explanation of the basic structure of the equation see tutorial `thfi`. The important difference to the tutorial `thfi` is that the Derjaguin pressure $-\partial_h f(h,x)$ now explicitly depends on the position x, i.e., we have a substrate that has a non-uniform wettability, i.e. the translational invariance is broken. Such a system was studied in [1, 2].
The technique introduced here was used in studies of droplets on heterogeneous inclined substrates [1, 2], and drops on the outside of rotating cylinders [3]. Related experiments and computer simulations are found in [4, 5].
Further, such 1d codes were employed in [6] where also 2d results obtained with other continuation codes are presented.

For the case without lateral driving see tutorial `hetdrop`. Here we assume a sinusoidal modulation of the long range contribution to the Derjaguin pressure:

$$\partial_h f(h,x) = -\Pi(h) = \frac{1}{h^3}\left[1 + \rho\sin(2\pi x/P)\right] - \frac{1}{h^6}. \tag{1.2}$$

where ρ and P are the relative strength and period of the heterogeneity. Note that the domain size L and the period of the heterogeneity are normally not identical. In a periodic setting one has $L = nP$ where $n > 0$ is an integer. Physically, the given form results in a modulation of equilibrium contact angle and precoursor film height.

To study steady solutions, i.e., resting droplets or modulated films, we set $\partial_t h = 0$ and integrate Eq. (1.1) once to obtain

$$0 \;=\; Q(h)\,\partial_x\left[\partial_{xx}h - \partial_h f(h,x)\right] + \chi(h) - C_0. \tag{1.3}$$

Here the constant C_0 stands for the mean flux that is constant for a steady solution. When writing Eq. (1.3) as a system of first-order ordinary differential equations on the interval $[0,\,1]$ (introducing $\xi = \frac{x}{L}\; u_1 = h - h_0$, $u_2 = dh/dx$ and $u_3 = d^2h/dx^2$), and using $\chi(h) = \alpha Q(h)$, then one obtains the non-autonomous system (r.h.s depends explicitly on x)

$$\begin{aligned}
\dot{u}_1 &= Lu_2\\
\dot{u}_2 &= Lu_3\\
\dot{u}_3 &= L\left[u_2 f_{u_1u_1}(u_1+h_0,x) + f_{u_1x}(u_1+h_0,x) - \alpha + \frac{C_0}{Q(u_1+h_0)}\right].
\end{aligned} \tag{1.4}$$

where L is the physical domain size, dots indicate derivatives with respect to ξ, and subscripts of f indicate partial derivatives. Such a non-autonomous system can not be handled by auto07p, therefore we transform it into an autonomous one. This is done by defining the position variable x to be another independent variable, i.e. $u_4 = x$ that as the other u_i depends on the independent variable ξ. One obtains the 4d dynamical system ($\mathrm{NDIM} = 4$)

$$\begin{aligned} \dot{u}_1 &= L(u_2 - \epsilon f_{u_1}(u_1 + h_0, u_4)) \\ \dot{u}_2 &= L(u_3 - \epsilon u_2) \\ \dot{u}_3 &= L\left[u_2 f_{u_1 u_1}(u_1 + h_0, u_4) + f_{u_1 u_4}(u_1 + h_0, u_4) - \alpha + \frac{C_0}{Q(u_1+h_0)}\right] \\ \dot{u}_4 &= L. \end{aligned} \tag{1.5}$$

Note that we have also introduced the unfolding parameter ϵ as in tutorial `drop`, it is needed for the first runs that use a horizontal substrate. We use periodic boundary conditions for u_1, u_2 and u_3 that take the form

$$u_1(0) = u_1(1), \tag{1.6}$$
$$u_2(0) = u_2(1), \tag{1.7}$$
$$u_3(0) = u_3(1). \tag{1.8}$$

As 4th BC we 'pin' the physical position $u_4 = x$ to the computational position ξ by

$$u_4(0) = 0, \tag{1.9}$$

(i.e., $\mathrm{NBC} = 4$). We also use an integral condition for mass conservation that takes the form

$$\int_0^1 u_1 \, \mathrm{d}\xi = 0; \tag{1.10}$$

and four integral conditions that measure various energies (see f.90 file; these could be removed and the code would still work, they are normalised w.r.t. the flat film starting solution). In the very first run that starts from a state which is invariant with respect to translation we also employ an integral condition that breaks this invariance, (see tutorial drop).
As starting solution we use a slightly sinusoidally perturbed flat film of height h_0 at zero driving ($\alpha = 0$), fix the domain size to its critical value $L = L_c$ and set $u_4 = L\xi$. Here $L_c = 2\pi/k_c$ where $k_c = \sqrt{-f''(h_0)}$ is the critical wavenumber for the linear instability of a flat film of thickness h_0 on the homogeneous substrate (see tutorial `drop`). The starting value for C_0 is zero as well as $\epsilon = 0$.

The number of free (continuation) parameters is given by

$$\underbrace{\mathrm{NCONT}}_{\text{no. of continuation par.}} = \underbrace{\mathrm{NBC}}_{\text{boundary conditions}} + \underbrace{\mathrm{NINT}}_{\text{integral conditions}} - \underbrace{\mathrm{NDIM}}_{\text{dimensionality}} + 1 \tag{1.11}$$

and is here equal to 7 or 6.

<table>
<tr><th>Python interface command line</th><th>Terminal command line</th></tr>
<tr><td>auto</td><td></td></tr>
<tr><td colspan="2">run 1: Compute the branch of periodic solutions for $h_0 = 3$, continue in domain size.
Continuation parameters: L (PAR(5)), C_0 (PAR(6)), ϵ (PAR(2)) and energies (PARs 36-38, 40), NINT= 6;
Settings: IPS= 4, ISP= 2, ISW= 1, ICP= $[5, 6, 2, 40, 35, 36, 37]$,
Start data from initial solution (IRS= 0) and check that ANZ= 1 in *.f90 file
Save output-files as b.h1, s.h1, d.h1. Plot continuation results for analysis.</td></tr>
<tr><td>r1 = run(e = ’hetdriv’, c = ’hetdriv.1’, sv = ’h1’)
plot(r1)</td><td>@@R hetdriv 1
@sv h1
@pp h1</td></tr>
<tr><td colspan="2">run 11: Compute branch of periodic solutions for $h_0 = 3$, $L = 50$ and continue in heterogeneity strength (ρ positive), starting from previous solution h1.
Continuation parameters: ρ (PAR(3)), C_0 (PAR(6)) , ϵ (PAR(2)) and energies (PARs 36-38, 40), NINT= 6;
Settings: IPS= 4, ISP= 2, ISW= 1, ICP= $[3, 6, 2, 40, 35, 36, 37]$.
Start data from LAB3 of run 1. Save output-files as <code>b.h11, s.h11, d.h11</code>.
Plot continuation results for analysis.</td></tr>
<tr><td>r11 = run(e = ’hetdriv’, c = ’hetdriv.11’, s = ’h1’, sv = ’h11’)
plot(r11)</td><td>@@R hetdriv 11 h1
@sv h11
@pp h11</td></tr>
<tr><td colspan="2">run 11b: Compute the branch of periodic solutions, same as run 11, but going towards negative heterogeneity strength ρ (PAR(3)); replace DS= 0.01 by DS= -0.01. Append current result (negative continuation) to previous result h11.
Plot continuation results for analysis.</td></tr>
<tr><td>r11b =r11 + run(e = ’hetdriv’, c = ’hetdriv.11b’,s = ’h11b’)
plot(r11b)</td><td>@@R hetdriv 11b h1
@ap h11
@pp h11</td></tr>
<tr><td colspan="2">run 111: Compute periodic solutions for $h_0 = 3$, $L = 50$, $\rho = 0.75$, continue in lateral driving α.
Continuation parameters: α (PAR(7)), C_0 (PAR(6)) and energies (PARs 36-38, 40), NINT= 5;
Settings: IPS= 4, ISP= 2, ISW= 1, ICP= $[7, 6, 40, 35, 36, 37]$.
start data from LAB18 of run 11. Save output-files as <code>b.h111, s.h111, d.h111</code> and plot results.</td></tr>
<tr><td>r111 = run(e =’hetdriv’,c = ’hetdriv.111’,s = ’h11’,sv = ’h111’)
plot(r111)</td><td>@@R hetdriv 111 h11
@sv h111
@pp h111</td></tr>
<tr><td>clean()</td><td>@cl</td></tr>
</table>

Table 1.1: Commands for running tutorial `hetdriv`.

1.2 Runs:

Run 1 Starting with a flat film on a homogeneous substrate ($\rho = 0$) without driving ($\alpha = 0$), determine steady solutions as a function of domain size L. Mean thickness $h_0 = 3$. We start at $L_c \approx 33$ and obtain profiles at domain sizes that are multiples of the heterogeneity period $P = 50$ (but heterogeneity remains switched off). (see fig.1.1,1.2.)

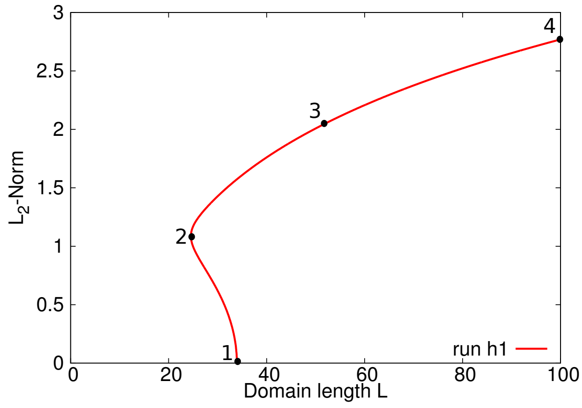

Figure 1.1: Graphic representation of the continuation of steady states with varying domain length L (PAR(5)). Shown is the Plot of the L2-norm vs domain length (**run h1**).

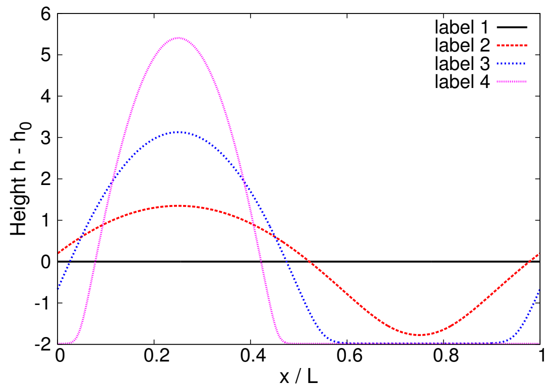

Figure 1.2: Shown are selected steady film profiles corresponding to the bifurcation curve in fig (1.1). (**run h1**).

Run 11 Starting with the drop solution at $L = 50$ on a homogeneous substrate ($\rho = 0$) without driving ($\alpha = 0$), determine steady solutions as a function of heterogeneity strength ρ (heterogeneity period $P = 50$). Mean thickness $h_0 = 3$ and domain size L is fixed.

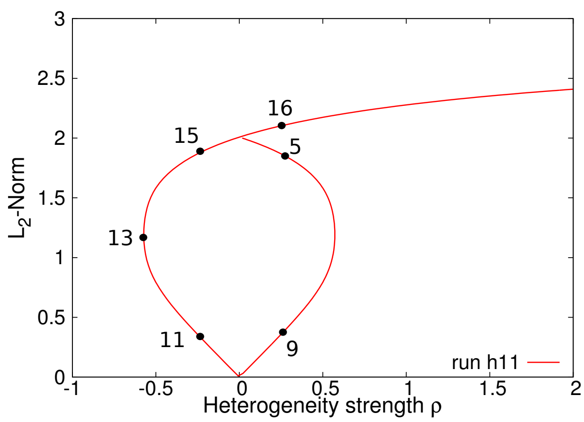

Figure 1.3: Plot of L_2-Norm vs. heterogeneity strength ρ.

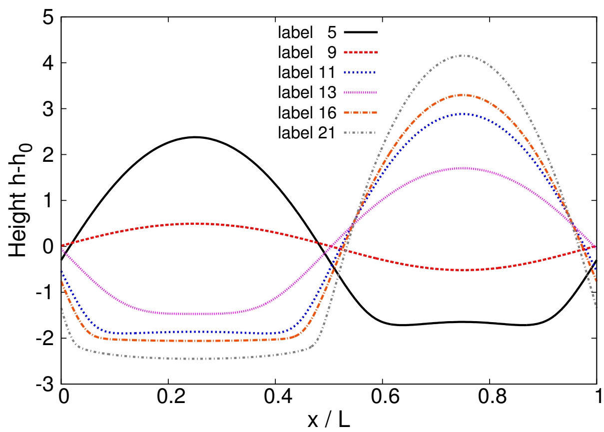

Figure 1.4: Selected Steady-state solutions corresponding to fig.(1.8).

Run 11b As run **11**, but going towards negative heterogeneity strength ρ. The following graphic shows the combination of run 11 and 11b.

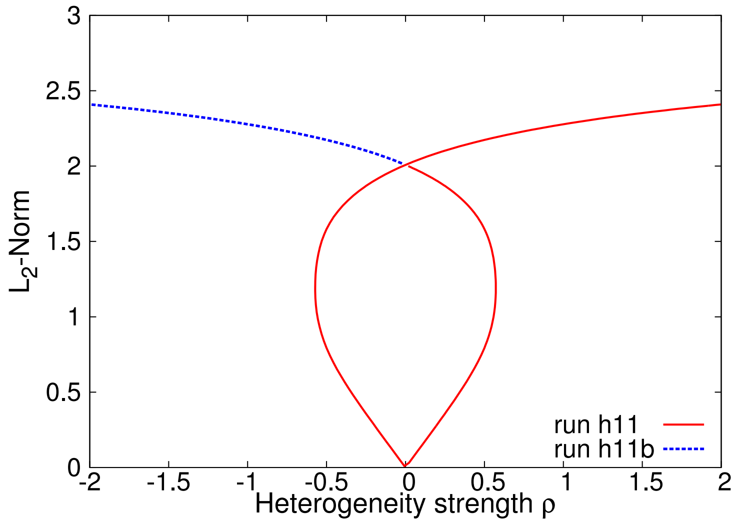

Figure 1.5: Combined results of run 11 and 11b.

Run 111 Starting with the drop solution at $L = 50$ on the heterogeneous substrate ($\rho = 0.75$) without driving ($\alpha = 0$), determine steady solutions as a function of lateral driving strength α ($P = L = 50$, $h_0 = 3$ and $\rho = 0.75$ fixed).

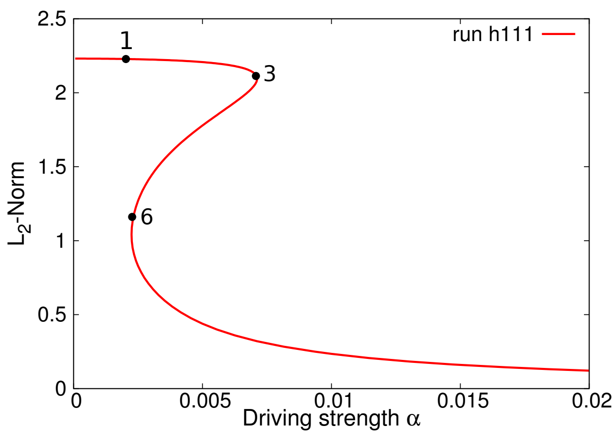

Figure 1.6: Graphical representation of L_2-Norm vs. driving strength α. A distinct film flattening can be observed for increased lateral driving strength (**run 111**).

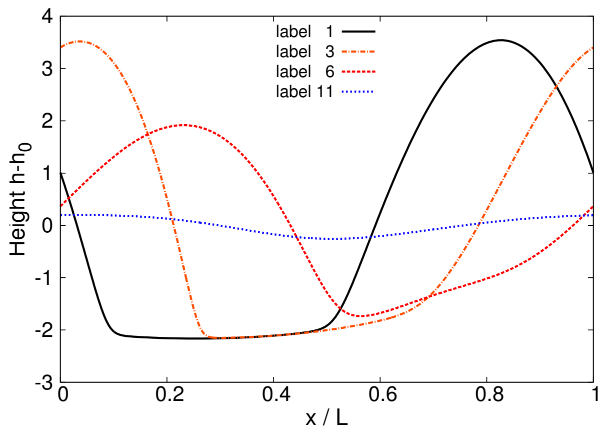

Figure 1.7: Selected profiles corresponding to the bifurcation curve of fig. (1.6)(**run 111**).

1.3 Remarks:

- Screen output and command line commands are also provided in README file, more info on continuation parameter in table. All runs also measure 4 energies.
- run 1 is in principle identical to run 1 in the tutorial `drop` but is here performed within a more complicated system of equations, which also describes heterogeneity and driving.
- The hetdriv.f90 file provides another 4 integral conditions that are used in all runs of the tutorial. They allow for a determination of the total energy of the obtained steady state solutions(PAR(40)), as well as of its components (surface energy(PAR(35)), wetting energy(PAR(36)) and potential energy(PAR(37))).
- The constant C_0 corresponds to the flow. (you may, for example, plot C_0 against the measured Energies with *@pp h111*)

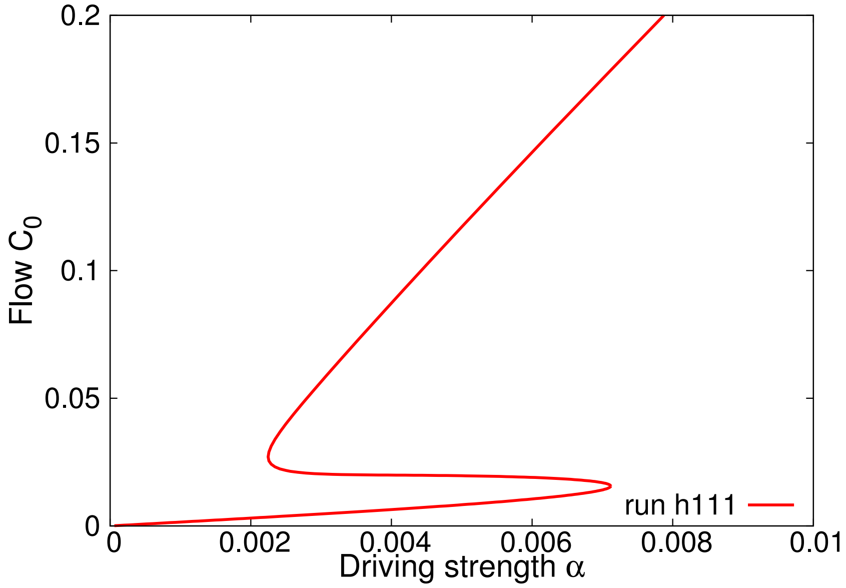

Figure 1.8: Plot of surface flow (C_0) vs. lateral driving parameter α.

1.4 Tasks:

After running the examples, you should try to implement your own adaptations, e.g.:

- Redo the runs for other values of h_0. What do you observe? (compare fig. 1.9)
- Deactivate the integral conditions that measures the energy of the solutions. (within subroutine ICND in .f90 file)
- Modulate the entire Derjaguin pressure instead of the long-range part (see eq.(1.1)). This corresponds to a modulation of the contact angle at fixed precursor film height.
- Replace the used Derjaguin pressure by a different one that you get from the literature (See tasks of tutorial `drop`).

- Look at two periods of the heterogeneity and get a full picture that shows what happens with all the solutions found in tutorial `hetdrop` under lateral driving (you may have to vary the period length, -number and the domain size in the .f90 file.)

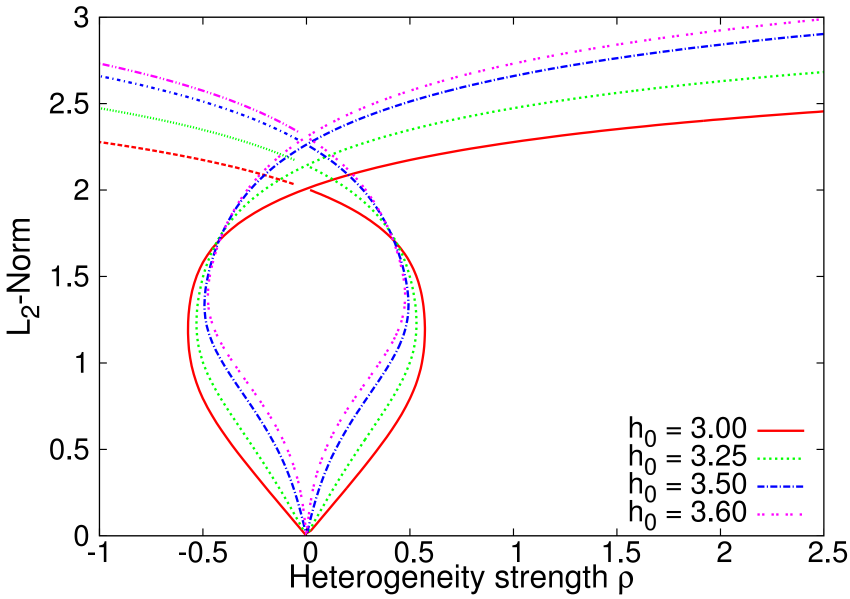

Figure 1.9: Plot of heterogeneity parameter ρ vs. L_2-Norm of steady state solution with different average film thicknesses H (h_0: 3.0 (red), 3.25 (blue), 3.5 (green), 3.75 (pink)).

References

[1] U. Thiele and E. Knobloch. On the depinning of a driven drop on a heterogeneous substrate. *New J. Phys.*, 8:313, 2006.

[2] U. Thiele and E. Knobloch. Driven drops on heterogeneous substrates: Onset of sliding motion. *Phys. Rev. Lett.*, 97:204501, 2006.

[3] U. Thiele. On the depinning of a drop of partially wetting liquid on a rotating cylinder. *J. Fluid Mech.*, 671:121–136, 2011.

[4] S Varagnolo, D Ferraro, P Fantinel, M Pierno, G Mistura, G Amati, L Biferale, and M Sbragaglia. Stick-slip sliding of water drops on chemically heterogeneous surfaces. *Phys. Rev. Lett.*, 111:066101, 2013.

[5] M Sbragaglia, L Biferale, G Amati, S Varagnolo, D Ferraro, G Mistura, and M Pierno. Sliding drops across alternating hydrophobic and hydrophilic stripes. *Phys. Rev. E*, 89:012406, 2014.

[6] P. Beltrame, E. Knobloch, P. Hänggi, and U. Thiele. Rayleigh and depinning instabilities of forced liquid ridges on heterogeneous substrates. *Phys. Rev. E*, 83:016305, 2011.